Advanced Computational Modeling for Reactor Design

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Summary

A variety of efforts at Argonne support and enable scientific research through mathematical modeling and simulation. These efforts leverage the substantial analytical expertise and the advanced computational technology developed at Argonne and allow researchers to probe regimes inaccessible to traditional experimental techniques. Recently these efforts have included the development of scalable parallel simulations in support of the design of the Very High Temperature Reactor being developed as a vehicle for clean hydrogen production on the large scale.

The Portable, Extensible Toolkit for Scientific computing (PETSc), developed at Argonne, is the premier scalable parallel numerical library, used in dozens of scientific applications around the world. PETSc helps bring the power of DOE's most advanced computational capabilities to both new and established scientific simulation codes. Key to PETSc's design is its encapsulation of the complexity of the underlying parallel numerical algorithms and its presentation of them in terms of the mathematical abstractions most familiar to scientists.

Recently PETSc was successfully applied in support of the design of the Very High Temperature Reactor at the Idaho National Laboratory (INL). Specifically, PETSc was used to extend the fully compressible flow codes, most notably the pressure-corrected implicit continuous Eulerian scheme (PCICE) developed at INL. Figure 1 illustrates the capabilities of PCICE at highly accurate resolution of compressible flows and heat transfer in complicated geometries. While PCICE is a state-of-the-art code capable of very accurate resolution of the wide range of fluid flows encountered in the core of a pebble-bed reactor, it lacks the parallel capabilities that would enable large-scale simulations. We have used PETSc to parallelize PCICE with minimal impact on the original code. Moreover, PCICE now has access to a variety of scalable linear solvers and flexible mesh manipulation tools offered by PETSc.

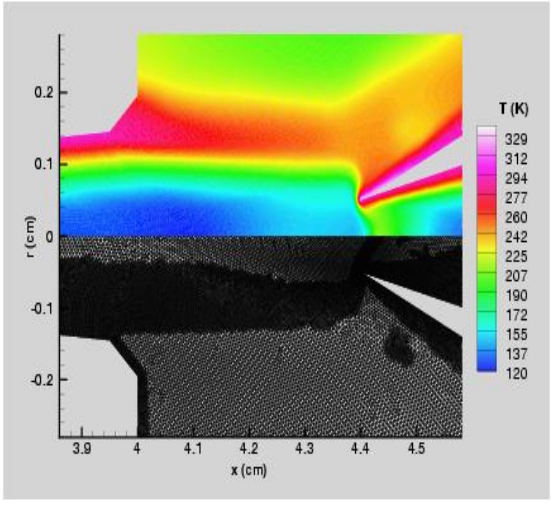

Figure 1. Temperature distribution obtained with PCICE in a nozzle subject to flow through it. Courtesy of Richard Martineau, INL.

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Extending PETSc's capabilities. Some of the capabilities introduced in our work with PCICE have necessitated extensions of PETSc to enable the handling of complicated geometric data, such as the structure of computational meshes and fields over them. To approach the additional complexity in a uniform way, we have introduced the notion of a *Sieve,* which abstracts the structure of topological objects, such as meshes, and extends it to more general hierarchical structures that can benefit from a geometric viewpoint.

The essential idea behind a Sieve is to consider a geometric object as composed, or covered by, more elementary subobjects. The utility of Sieves lies in their ability to manipulate distributed decompositions of arbitrary complexity in a scalable way presented in a concise interface. The numerical data attached to Sieves, such as the pressure and temperature fields defined over computational meshes, are regarded as the *sections* of a *fiber bundle* over the Sieve, to borrow a term from differential geometry. The analogy is more than just terminological: the decomposition of a Sieve allows us to define the restriction and prolongation operations on the data, so that computations can proceed in the local setting of a subobject, and later be automatically reassembled.

Applications. We anticipate that the newly introduced capabilities will help, not only in the scalable parallelization of PCICE, but also in its coupling to the EVENT neutronics code from Georgia Tech, completing an essential kernel of a reactor simulation. Further advantages include the ability to implement flexible parallel adaptive mesh refinement and load-balancing strategies using only a serial mesh generator and the mesh improvement algorithms also developed at Argonne.

In addition to reactor design applications we envision using Sieves and PETSc's geometric capabilities in general to analyze the structure of large genetic and metabolic networks. We anticipate the development of metabolic engineering tools for the maximization of flux through critical metabolic pathways, such as those responsible for the hydrogen production in bacteria.

Furthermore, scalable parallel codes for hierarchical nonlocal field computations, such as those encountered in micromagnetics and electrostatics, will greatly benefit from the powerful topological abstractions. They are based on multipole expansions or the interaction kernel interpolation, whose implementation can be simplified into many cooperating Sieves. Moreover, the nontrivial global topology of micromagnetic formulations is also easy to incorporate.

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